

# Chemistry Cheatsheet

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partly based on the work by L. Hoffmann & D. Vermeer

Version: November 1, 2023

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## 1. Basics

### 1.1 Unit conversions

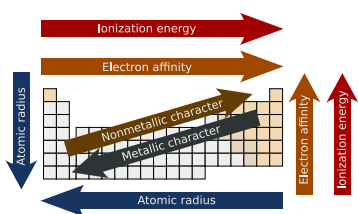
- Energy:**  $1\text{eV} = 1.602 \cdot 10^{-19}\text{J}$ ,  $1\text{cal} = 4.18\text{J}$
- Pressure:**  $P = \frac{F}{A} = \rho \cdot h \cdot g$   
 $1\text{atm} = 760\text{mm Hg} = 760\text{torr} = 101'325\text{Pa} = 1.01325\text{bar}$   
Manometer:  $P = P_{\text{atm}} \pm \rho gh$
- Force:**  $F = m \cdot g$ ,  $m = \rho \cdot V$
- Amount of substance:**  $1\text{mol} = 6.022 \cdot 10^{23}$  (Avogadro)
- Length:**  $1\text{\AA} = 10^{-10}\text{m}$
- STP:**  $0^\circ\text{C} = 273.15\text{K}$ ,  $1\text{atm}$ ;  $V_m = 22.41\text{L}$

### 1.2 General

- Kinetic energy:**  $E_{\text{kin}} = \frac{1}{2} \cdot m \cdot v^2$
- Potential energy:**  $E_{\text{pot}} = m \cdot g \cdot \Delta h$
- electrostatic:**  $E_{\text{el}} = \frac{\kappa Q_1 Q_2}{d^2}$ ,  $\kappa = \frac{1}{4\pi\epsilon_0}$
- Photon energy:**  $E_\gamma = h \cdot f = \frac{h \cdot c}{\lambda}$
- De Broglie wavelength:**  $\lambda = \frac{h}{m \cdot v}$

### 1.3 Trends in the periodic table of elements

- Ionisation energy:** The ionization energy is the quantity of energy that an isolated, gaseous atom in the ground electronic state must absorb to discharge an electron, resulting in a cation.
- Electron affinity:** Electron affinity is defined as the change in energy (in kJ/mole) of a neutral atom (in the gaseous phase) when an electron is added to the atom to form a negative ion.
- Electronegativity:** Electronegativity is a measure of an atom's ability to attract shared electrons to itself.



## 2. Atoms

### 2.1 Quantum mechanics

Atomic mass = total mass  
Atomic weight = average atomic mass (isotopes)  
Atomic number = #protons  
mass number = #protons + #neutrons

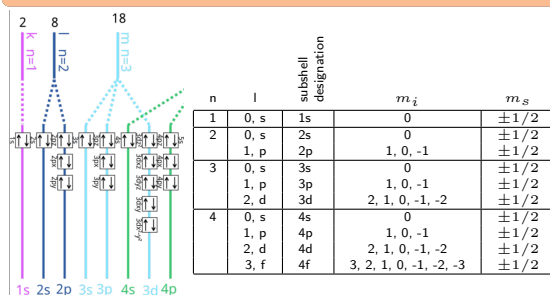
Heisenbergs uncertainty principle  $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$ . Due to duality of electrons (acting like waves and elementary entities at the same time), impossible to exactly describe position and momentum simultaneously.

**Effective nuclear charge (approx.):**  $Z_{\text{eff}} = Z - S$

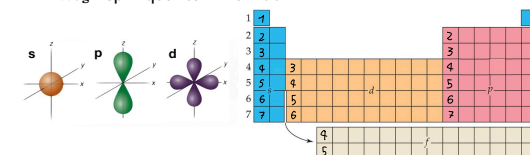
$Z$  = #protons,  $S$  = # $e^-$  on all full shells

In periodic table:  $Z_{\text{eff}}$  increases from left to right  $\rightarrow$  electrons are more attracted and hence atomic radius is smaller, the further right in the periodic table. ( $e^-$  repulsion vs. nuclear charge)

### 2.2 Orbitals



- n:** principal quantum number  $\rightarrow$  size of orbital
- l:** angular quantum number  $\rightarrow$  shape of orbital
- $m_l$ :** magnetic quantum number  $\rightarrow$  orientation of orbital
- $m_s$ :** spin quantum number



Pauli Exclusion: Each electron has unique set of quantum numbers  
Hund's rule: **Every** orbital in sublevel is first singly occupied  
Energy of Hydrogen  $e^-$ :  $E_n = -\frac{hcR_H}{n^2}$ ,  $R_H = 1.097 \cdot 10^7\text{m}^{-1}$   
Excitement from shell  $n_1$  to  $n_2$ :  $E_H = hcR_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$

## 3. Chemical bondings

### 3.1 Covalent bondings

Two atoms share electron pairs  
**octet rule:** Atom tries to acquire noble state (2 valence electrons for H and He, 8 valence electrons for all other)  
**exceptions:**

- Odd electrons
- Less / more than 8 VE's on central atom

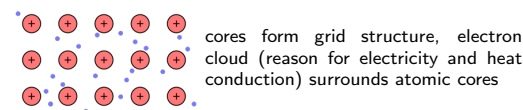
### 3.2 Lewis structure

- Write symbols and connect with single bonds
- Complete octets around non-central atoms
- Place remaining VE around central atom
- Try multiple bonds if central atom does not have octet
- if multiple lewis structures possible: choose most stable according to formal charge

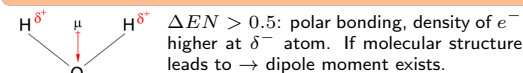
### 3.3 Ionic bonding

Electrons transferred from atoms with lower EN to atoms with higher EN  $\rightarrow$  cations (+) (smaller radius) and anions (-) (bigger radius). electrostatic attraction.  $\Delta EN > 1.7 \rightarrow$  ionic bonding  
lattice energy  $\Delta U$ : Energy to separate ions to infinite distance  
**Born Haber Cycle:**  $AB \rightarrow A^+ + B^-$  Visualization of calculation of  $\Delta U$ :  $\Delta H_f[AB] + \Delta I[A] - \Delta EA(B)$ , A & B in **gaseous** state

### 3.3 Metallic bonding



### 3.4 Polarity and Dipole moment



### 3.5 Formal charges

Results if new bondings are formed to satisfy octet rule, ignores electronegativity.

$$\text{Formal charge} = \left[ \text{atom's v.e.s} \right] - \frac{1}{2} \cdot \left[ \text{bonding e.s} \right] - \left[ \text{nonbonding e.s} \right]$$

### 3.6 Bonding strength and length

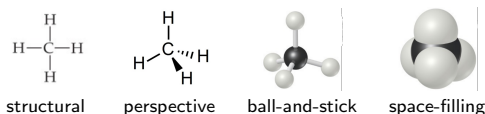
**Bond length:**  $\equiv < < -$       **Bond strength:**  $- < < \equiv$

**Bond enthalpy** = [broken bonds] - [formed bonds]

**Most stable molecule:**

- least formal charges.
- formal charges necessary: choose smallest effective charge of molecule (sum of formal charges)
- negative formal charge on electronegative atom

## 4. Molecular models



### 4.1 valence shell electron pair repulsion (VSEPR)

Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry		
		No Lone Pairs	1 lone Pair	2 lone Pairs
2	Linear 180°	Linear		
3	Trigonal planar 120°	Trigonal planar	Bent	
4	Tetrahedral 109°	Tetrahedral	Trigonal pyramidal	Bent
5	Trigonal bipyramidal 120°/90°	Trigonal bipyramidal	Seesaw	T-shaped
6	Octahedral 90°	Octahedral	Square pyramidal	Square planar

## 5. State of matter

### 5.1 Intermolecular forces

- Van-der-Waals interactions** (weak)

#### (a) Dipol-Dipol

Sum of all dipole moments from polar bonds in molecule. (molecular dipole) ( $\Delta EN > 0.5$ )

#### (b) Dispersion

Temporary fluctuations of the electrons can cause an induced dipole. **These forces always exist.** Force increases with molecule size and also affected by molecular shape.

- Ion-Dipole Interactions** (strong)

Very important for solutions. Ions solvated by polar liquid.

- Hydrogen bonding** (strong)

One type of dipole-dipole interaction. N, O, F are very electronegative  $\Rightarrow$  very polar bonds with H.

Ion-Dipole > H-Bonding > Dipole-Dipole  $\approx$  Dispersion  
50kJ/mol      ~ 25kJ/mol      ~ 50kJ/mol

### 5.2 Fluids

**Colligative Properties:** Changes depend on amount of solute added, but not which solute.

$$\text{Clausius-Clapeyron} \left\{ \begin{array}{l} \ln(P_{\text{vap}}) = -\frac{\Delta H_{\text{vap}}}{RT} + C \\ \ln\left(\frac{P_1}{P_2}\right) = \frac{\Delta H_{\text{vap}}}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \end{array} \right.$$

### Boiling-Point Elevation:

$$\Delta T_b = T_b(\text{solution}) - T_b(\text{solvent}) = iK_b m$$

$m$  = molality of solute

$K_b$  = molal bp elevation constant (solvent)

$i$  = van't Hoff factor

= 1 for non-electrolytes

= Number of ions produced for electrolytes. e.g 2 for NaCl

### Vapor-Pressure Lowering:

$$P_{\text{vap}}^{\text{sol}} = X_{\text{solvent}} \cdot P_{\text{vap}}^{\text{pure}}$$

Raoult's law — Solution is an ideal solution. All intermolecular interactions are identical.

### Freezing-Point Depression:

$$\Delta T_f = T_f(\text{solution}) - T_f(\text{solvent}) = -iK_f m$$

$m$  = molality of solute = (moles of solute)/(kg of solvent)

$K_f$  = molal fp depression constant (solvent)

$i$  = van't Hoff factor

## 5.3 Expressions for Solutions

- $X$  Mole fraction =  $\frac{\text{moles solute or solvent}}{\text{total moles}}$
- $M$  Molarity =  $\frac{\text{moles solute}}{\text{litres solution}}$
- $m$  Molality =  $\frac{\text{moles solute}}{\text{kg solvent}}$
- Mass% =  $\frac{\text{mass solute}}{\text{total mass}} \cdot 10^2$ , ppm:  $\cdot 10^6$ , ppb:  $\cdot 10^9$

## 5.4 Ideal Gas

- Assumptions of IGL
  - Gas molecules don't occupy much of total volume.
  - Gas molecules don't interact.

- Ideal Gas Law:  $PV = nRT = NkT$
- $P$  [Pa],  $V$  [ $\text{m}^3$ ],  $n$  [num of moles],  $R$  [ $\frac{\text{J}}{\text{mol} \cdot \text{K}}$ ],  $T$  [K]
- Density  $\rho = M \cdot \frac{n}{V} = M \cdot \frac{P}{RT}$

### Partial pressure:

$$P_i = n_i \cdot \frac{RT}{V} \quad \text{total pressure} = \sum \text{of all partial pressures.}$$

### Henry's law:

$$S_g = kP_g$$

$P_g$  = Partial Pressure above liquid  
 $k$  = Henry's law constant

## 5.5 Osmotic pressure

Pressure needed to counteract osmotic flow.

$$\Pi = i \left( \frac{n}{V} \right) RT = iMRT$$

## 6. Thermodynamics

### 6.1 System types

- Open** Can exchange matter and energy w/ surrounding
- Closed** Can exchange energy w/ surrounding
- Isolated** Nothing can be exchanged
- intensive** independent, **extensive** dependent of system size

### 6.2 E = Internal energy of system

- $\Delta E = E_{\text{final}} - E_{\text{initial}}$   
 $\Delta E > 0$  system gained energy  
 $\Delta E < 0$  system lost energy
- 1st Law of Thermodynamics**  
 $\Delta E = q + w = q_V$  (constant V)  
 $q$  = heat added to system,  $w$  = work done on system

## 6.3 Enthalpy, $H$

$\Delta H$  tells us about heat transferred during chemical reaction.

- $\Delta H = \Delta E + \Delta(PV) = q_p$  heat flow at constant  $P$
- $w = -P\Delta V$  = pressure-volume work =  $-\Delta nRT$
- $\Delta H > 0 \Rightarrow$  endothermic
- $\Delta H < 0 \Rightarrow$  exothermic

## 6.4 Heat Capacity

Heat flow required to raise substance's  $T$  by 1 degree  $^{\circ}C$  (or  $K$ )

$$C_m = \text{molar heat capacity} = \left[ \frac{J}{\text{mol}^{\circ}C} \right] = \left[ \frac{J}{\text{mol} K} \right]$$

$$C_s = \text{specific heat capacity} = \left[ \frac{J}{g^{\circ}C} \right] = \left[ \frac{J}{g K} \right]$$

Ex.  $q = C_m \cdot n \cdot \Delta T = C_s \cdot m \cdot \Delta T =$  Heat of vaporization

**Hess's Law:**  $\Delta H_{rxn} = \sum \Delta H_i$

e.g Enthalpies of Formation:  $\Delta H_f^{\circ}$

## 6.5 Entropy, $S$

Entropy is a measure of disorder in a system. All spontaneous processes are irreversible.  $S$  is a state function.

- $\Delta S = \frac{q_{rev}}{T}$ ,  $q_{rev}$  = heat flow for reversible process
- $S = k_b \cdot \ln(W)$ ,  $k_b$  = Boltzmann's constant,  $W$  = num of microstates

$\Delta S > 0$ : increasing microstates

e.g increasing  $V$ , increasing  $T$ , increasing  $n$ , increasing complexity of molecules, melting solids, vaporizing liquids, mixing gases

## 6.6 2nd Law of Thermodynamics

Entropy of the universe increases for any spontaneous process.

$$\Delta S_{univ} = \Delta S_{sys} + \Delta S_{surr} > 0 \text{ (spontaneous, irreversible)}$$

$$\Delta S_{univ} = \Delta S_{sys} + \Delta S_{surr} < 0 \text{ (nonspontaneous)}$$

$$\Delta S_{univ} = \Delta S_{sys} + \Delta S_{surr} = 0 \text{ (reversible)}$$

## 6.7 Gibbs Free Energy

$$G = H_{sys} - T \cdot S_{sys} \text{ at constant } T$$

$\Delta H$	$\Delta S$	$-T\Delta S$	$\Delta G$	Reaction Characteristics
-	+	-	-	at all $T$ Spontaneous
+	-	+	+	at all $T$ Nonspontaneous
-	+	-	+or-	$\downarrow T$ Spon.; $\uparrow T$ Nonsp.
+	+	-	+or-	$\downarrow T$ Nonsp.; $\uparrow T$ Spon.

## 7. Kinetics

### 7.1 Reaction rate

Given general rxn:  $\alpha A + \beta B \rightarrow \gamma C + \delta D$

$$0 < \text{Rate} = -\frac{1}{\alpha} \frac{d[A]}{dt} = -\frac{1}{\beta} \frac{d[B]}{dt} = \frac{1}{\gamma} \frac{d[C]}{dt} = \frac{1}{\delta} \frac{d[D]}{dt}$$

Rate of disappearance of reactants      Rate of appearance of products

### 7.2 Rate Law

$$\text{Rate} \left[ \frac{M}{s} \right] = k[A]^m[B]^n$$

- rate only depends on reactants
- $k$  is the rate constant
- $m, n$  are the reaction orders
- $m, n$  can be 0,  $\frac{1}{2}$ , 1, 2, ...
- $m + n$  is overall rxn order
- $m, n$  are not necessarily equal to  $\alpha, \beta$

## 7.3 Reaction Orders

Consider  $A \rightarrow B$

$[A]_t$  = concentration of  $A$  at time  $t$

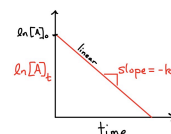
$[A]_0$  = concentration of  $A$  at time  $t = 0$

### 1st Order

$$\text{Rate} = -\frac{d[A]}{dt} = k[A]^1$$

$$\ln[A]_t = -kt + \ln[A]_0$$

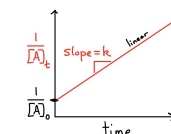
$$[A]_t = [A]_0 \cdot \exp(-kt)$$



### 2nd Order

$$\text{Rate} = -\frac{d[A]}{dt} = k[A]^2$$

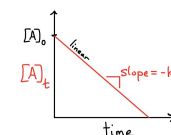
$$\frac{1}{[A]_t} = kt + \frac{1}{[A]_0}$$



### Zero Order

$$\text{Rate} = -\frac{d[A]}{dt} = k[A]^0 = k$$

$$[A]_t = -kt + [A]_0$$



### 7.4 Half Life

Time needed for  $[A]_t = \frac{1}{2}[A]_0$

$$\begin{matrix} t_{\frac{1}{2}} = \frac{0.693}{k} & t_{\frac{1}{2}} = \frac{1}{k[A]_0} & t_{\frac{1}{2}} = \frac{[A]_0}{2k} \\ \text{1st Order} & \text{2nd Order} & \text{Zero Order} \end{matrix}$$

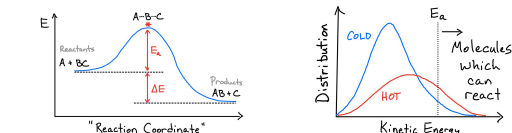
### 7.5 Collision Model

Reaction requires reactant molecules to collide with correct orientation and enough energy.

Higher  $T$ : reactants collide more often and with more kinetic  $E$ .

**Arrhenius**

Molecules need minimum energy to react; Activation Energy,  $E_a$



### 7.6 Arrhenius Equation

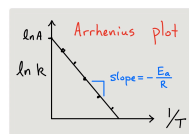
$$\alpha A + \beta B + \gamma C \rightarrow \text{products} \quad \text{Rate} = k[A]^m[B]^n[C]^p$$

$$k(T) = \underbrace{\left( \frac{\text{collisions}}{\text{per time}} \right)}_A \cdot \underbrace{\left( \frac{\text{fraction of collisions properly oriented}}{\text{properly oriented}} \right)}_B \cdot \underbrace{\left( \frac{\text{fraction of molecules with } E > E_a}{\text{with } E > E_a} \right)}_C \cdot \exp\left[ \frac{-E_a}{RT} \right]$$

$A$  is a "frequency factor", assumed  $T$ -independent

$$\ln(k) = \frac{-E_a}{R} \cdot \frac{1}{T} + \ln(A)$$

$$\ln\left(\frac{k_1}{k_2}\right) = \frac{-E_a}{R} \cdot \left( \frac{1}{T_1} - \frac{1}{T_2} \right)$$



### 7.7 Reaction Mechanisms

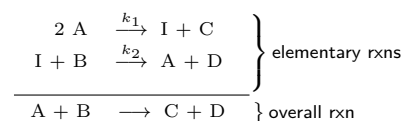
A sequence of elementary rxns that sum to the overall rxn. The kinetics of elementary rxns are determined by how many molecules have to collide, referred to as the molecularity.

Elementary rxns have rate law where  $m, n, p, \dots$  are equal to stoichiometric coefficients.

Molecularity	Elementary rxn	Rate law
Unimolecular	$A \rightarrow P$	$k[A]$
Bimolecular	$A + A \text{ or } A + B \rightarrow P$	$k[A]^2$
Termolecular	$A + A + B \text{ or } \dots \rightarrow P$	$k[A]^2[B]$

### 7.8 Multistep Reactions

Overall rate law results from the individual rate laws for the individual elementary reactions.



Assume  $k_1 \ll k_2$ , i.e. step 1 is "rate limiting"

$\Rightarrow$  rate overall =  $k_1[A]^2$

### 7.9 Catalysts

Substances that increase rxn rate, but are neither produced nor consumed in overall rxn.

Can  $\begin{cases} \text{increase } A & \Rightarrow \text{better orient molecules} \\ \text{lower } A & \Rightarrow \text{lower energy of transition state or} \\ & \text{allow new mechanism} \end{cases}$

Lower  $E_a$  has bigger impact

$\Rightarrow$  Appears in exponent of  $k(T) = A \cdot \exp\left(\frac{-E_a}{RT}\right)$

### 8. Chemical Equilibrium

$A \xrightleftharpoons[k_r]{k_f} B$ , at equilibrium:  $\text{Rate} = k_f[A] = k_r[B]$ ;  $\frac{[B]}{[A]} = \frac{k_f}{k_r}$

### 8.1 Law of mass action, equilibrium-constant

molarity concentrations      partial pressures ( $\text{bar} = \text{kJ/mol} \cdot 10^{-2}$ )

$$K_c = \frac{[C]^{\gamma}[D]^{\delta}}{[A]^{\alpha}[B]^{\beta}} \quad K_p = \frac{[P_C]^{\gamma}[P_D]^{\delta}}{[P_A]^{\alpha}[P_B]^{\beta}} = K_c(RT)^{\Delta n}$$

$K \gg 1 \rightarrow$  products dominate,  $K \ll 1 \rightarrow$  reactants dominate  
 $K$  depends on  $T$  and is unitless

**heterogeneous equilibria:** exclude pure solids / liquids from  $K$   
reaction quotient  $Q$  if not at equilibrium, calculated like  $K_c$

- rxn written in reverse:  $K = K_{\text{original}}^{-1}$
- rxn multiplied by  $n$ :  $K = (K_{\text{original}})^n$
- multistep rxn:  $K = K_1 \cdot K_2 \cdot K_3 \dots$
- With catalysts: equilibrium is reached faster,  $K$  unchanged

### 8.2 Le Châtelier's principle

**Disturbance in concentration**

system reacts to consume added substance



**Disturbance in pressure**

reduced volume  $\rightarrow$  system shifts in direction with fewer moles of gas

**Disturbance in temperature**

**Endothermic**  
increased  $T$       right shift  
decreased  $T$       left shift

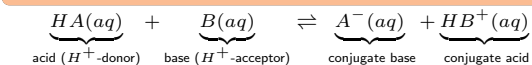
**Exothermic**  
left shift  
right shift

### 8.3 Connection to Thermodynamics

$$\Delta G^{\circ} = -RT \cdot \ln(K) \quad \text{or} \quad K = \exp\left(\frac{-\Delta G^{\circ}}{RT}\right)$$

## 9. Acid Base Reactions

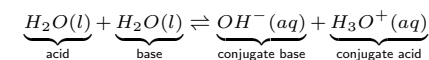
### 9.1 Brownsted Lowry acids and bases



strong acids/bases completely ionize, weak acids/bases don't

## 9.2 Autoionisation of water

Amphiprotic substances (ex. Water) can act as acid and base



$$K_w \equiv K_C = [OH^-][H_3O^+] = 10^{-14} (25^{\circ}C)$$

### 9.3 Reaction of acid with water / base with water

$$\text{acid-dissociation} \quad K_a \equiv K_C = \frac{[A^-][H_3O^+]}{[HA]} \quad \text{base-dissociation} \quad K_b \equiv K_C = \frac{[HB^+][OH^-]}{[B]}$$

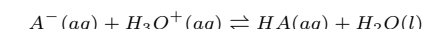
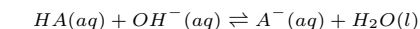
### 9.4 p-Scales

$$p(\xi) = -\log(\xi) \quad pH = -\log[H_3O^+] \quad pOH = -\log[OH^-]$$

$pH + pOH = 14$        $pH < 7 \rightarrow$  acid       $pH > 7 \rightarrow$  base

### 9.5 common ion effect and Buffers

$CH_3COOH + CH_3COONa \rightarrow$  dissociates to  $CH_3COO^-$



$$[H_3O^+] = K_a \frac{[HA]}{[A^-]} \rightarrow pH_{\text{buffer}} = pK_a + \log\left(\frac{[base]}{[acid]}\right)$$

For disturbance small relative to  $[HA]$ ,  $[A^-] \rightarrow$  small  $pH$  change

## 10. Redox Reactions (electron transfer)

### 10.1 Oxidation Numbers

- Atoms in elemental form: **0**
- Monoatomic ions: **ionic charge**
- Nonmetals in ionic/molecular compounds: **negative oxidation numbers**
  - Oxygen: -2 (except peroxide ion,  $O_2^{2-}$ , -1)
  - H: +1 (except if bonded to metal, -1)
  - F: -1 (always)
  - Cl, Br, I: -1 (except if bonded to oxygen)
- Sum of oxidation numbers for atoms in compound equals its net charge

### 10.2 Energy and Batteries

- Cathode  $\oplus$ : reduction
- Anode  $\ominus$ : oxidation
- Anions  $\rightarrow$  anode
- Cations  $\rightarrow$  cathode

Electric potential = potential energy difference per unit charge

$$1V = \frac{1.6 \cdot 10^{-19} J}{1.6 \cdot 10^{-19} C}$$

$$E_{\text{cell}}^{\circ} \equiv \text{Cell voltage at standard conditions}$$

$$E_{\text{red}}^{\circ} \equiv \text{Potential energy available if reduced}$$

$$\text{Cell potential} \Rightarrow E_{\text{cell}}^{\circ} = E_{\text{red}}^{\circ}(\text{cathode}) - E_{\text{red}}^{\circ}(\text{anode})$$

### 10.3 Connection to Gibbs Free Energy

$$\Delta G^{\circ} = -nFE_{\text{cell}}^{\circ} \quad \Delta G^{\circ} = J/\text{mol of rxn}$$

$F$  = Faraday's constant

$$E_{\text{cell}}^{\circ} > 0, \Delta G^{\circ} < 0 \quad n = \text{unitless number moles of } e^- \text{'s transferred in balanced cell rxn}$$

$\Rightarrow$  **Spontaneous!**

### 10.4 Balance Redox reactions

acidic soln	basic soln
Divide into oxidation- and reduction half-rxn	Divide into oxidation- and reduction half-rxn
Balance all elements, Balance $H$ and $O$ by adding $H_3O^+$ and $H_2O$ , add required $e^-$	"Neutralize" $H^+$ with $OH^-$ , form $H_2O$ , cancel $H_2O$ on both sides
Multiply half rxns by integers to equate electrons	Multiply half rxns by integers to equate electrons
Add half rxns together	Add half rxns together
Check balance	Check balance